M Vernica Ganduglia-Pirovano

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104 papers	6,771 citations	42 h-index	81 g-index
114 ext. papers	7,483 ext. citations	5.9 avg, IF	5.98 L-index

#	Paper	IF	Citations
104	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. *Surface Science Reports*, **2007**, 62, 219-270	12.9	982
103	Hybrid functionals applied to rare-earth oxides: The example of ceria. *Physical Review B*, **2007**, 75,	3.3	461
102	Density-functional calculations of the structure of near-surface oxygen vacancies and electron localization on CeO2(111). *Physical Review Letters*, **2009**, 102, 026101	7.4	442
101	Dry Reforming of Methane on a Highly-Active Ni-CeO2 Catalyst: Effects of Metal-Support Interactions on C-H Bond Breaking. *Angewandte Chemie - International Edition*, **2016**, 55, 7455-9	16.4	196
100	Catalysis and corrosion: the theoretical surface-science context. *Surface Science*, **2002**, 500, 368-394	1.8	186
99	Role of ceria in oxidative dehydrogenation on supported vanadia catalysts. *Journal of the American Chemical Society*, **2010**, 132, 2345-9	16.4	171
98	Raman Spectra of Polycrystalline CeO2: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2017**, 121, 20834-20849	3.8	157
97	In situ and theoretical studies for the dissociation of water on an active Ni/CeO2 catalyst: importance of strong metal-support interactions for the cleavage of O-H bonds. *Angewandte Chemie - International Edition*, **2015**, 54, 3917-21	16.4	155
96	Role of subsurface oxygen in oxide formation at transition metal surfaces. *Physical Review Letters*, **2002**, 89, 096103	7.4	154
95	Electronic and nuclear chemical reactivity. *Journal of Chemical Physics*, **1994**, 101, 8988-8997	3.9	150
94	Surface core-level shifts of clean and oxygen-covered Ru(0001). *Physical Review B*, **2001**, 63,	3.3	144
93	Electron localization in defective ceria films: a study with scanning-tunneling microscopy and density-functional theory. *Physical Review Letters*, **2011**, 106, 246801	7.4	140
92	Resolving the atomic structure of vanadia monolayer catalysts: monomers, trimers, and oligomers on ceria. *Angewandte Chemie - International Edition*, **2009**, 48, 8006-9	16.4	127
91	Structural and electronic properties of chemisorbed oxygen on Rh(111). *Physical Review B*, **1999**, 59, 15533-15543	3.3	120
90	Metastable precursors during the oxidation of the Ru(0001) surface. *Physical Review B*, **2002**, 65,	3.3	112
89	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. *Chemical Physics Letters*, **2002**, 352, 311-317	2.5	111
88	Stability of reduced V2O5(001) surfaces. *Physical Review B*, **2004**, 70,	3.3	110

87	Room-Temperature Activation of Methane and Dry Re-forming with CO2 on Ni-CeO2(111) Surfaces: Effect of Ce3+ Sites and Metal□Support Interactions on C□H Bond Cleavage. *ACS Catalysis*, **2016**, 6, 8184-8191	12.1	105
86	Evidence for subsurface ordering of oxygen vacancies on the reduced CeO2(111) surface using density-functional and statistical calculations. *Physical Review Letters*, **2013**, 110, 246101	7.4	101
85	Insight into the Adsorption of Water on the Clean CeO2(111) Surface with van der Waals and Hybrid Density Functionals. *Journal of Physical Chemistry C*, **2012**, 116, 13584-13593	3.8	99
84	Reactivity kernels, the normal modes of chemical reactivity, and the hardness and softness spectra. *Journal of Chemical Physics*, **1995**, 103, 3543-3551	3.9	99
83	Surface metal-insulator transition on a vanadium pentoxide (001) single crystal. *Physical Review Letters*, **2007**, 99, 226103	7.4	98
82	Molecular-Level Understanding of CeO2 as a Catalyst for Partial Alkyne Hydrogenation. *Journal of Physical Chemistry C*, **2014**, 118, 5352-5360	3.8	92
81	Hydrogen activation, diffusion, and clustering on CeO□(111): a DFT+U study. *Journal of Chemical Physics*, **2014**, 141, 014703	3.9	92
80	In Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal-Support Interactions and C-H Bond Activation at Low Temperature. *Angewandte Chemie - International Edition*, **2017**, 56, 13041-13046	16.4	90
79	Counting electrons transferred through a thin alumina film into Au chains. *Physical Review Letters*, **2008**, 100, 096802	7.4	90
78	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. *Surface Science*, **1999**, 422, 8-16	1.8	88
77	Theoretical Studies of the Adsorption of CO and C on Ni(111) and Ni/CeO2(111): Evidence of a Strong Metal□Support Interaction. *Journal of Physical Chemistry C*, **2013**, 117, 8241-8250	3.8	86
76	Direct Conversion of Methane to Methanol on Ni-Ceria Surfaces: Metal-Support Interactions and Water-Enabled Catalytic Conversion by Site Blocking. *Journal of the American Chemical Society*, **2018**, 140, 7681-7687	16.4	84
75	Comment on □aming multiple valency with density functionals: A case study of defective ceria□ *Physical Review B*, **2005**, 72,	3.3	81
74	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. *Physical Review B*, **2004**, 69,	3.3	70
73	Oxygen-induced Rh 3d5/2 surface core-level shifts on Rh(111). *Physical Review B*, **2001**, 63,	3.3	69
72	Formaldehyde formation on vanadium oxide surfaces V2O3(0001) and V2O5(001): how does the stable methoxy intermediate form?. *Angewandte Chemie - International Edition*, **2009**, 48, 3695-8	16.4	56
71	Formation of the cerium orthovanadate CeVO4: DFT+U study. *Physical Review B*, **2007**, 76,	3.3	56
70	Ordering of oxygen vacancies and excess charge localization in bulk ceria: A DFT+U study. *Physical Review B*, **2014**, 90,	3.3	55

69	Periodic Density Functional Theory Study of VOn Species Supported on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 7399-7410	3.8	52
68	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. *Topics in Catalysis*, **2008**, 50, 106-115	2.3	52
67	Potential, core-level, and d band shifts at transition-metal surfaces. *Physical Review B*, **1996**, 54, 8892-8898	3.3	52
66	Orbital symmetry, reactivity, and transition metal surface chemistry. *Physical Review Letters*, **1994**, 72, 3222-3225	7.4	52
65	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. *Surface Science*, **2006**, 600, 1497-1503	1.8	50
64	Adlayer core-level shifts of admetal monolayers on transition-metal substrates and their relation to the surface chemical reactivity. *Physical Review B*, **1996**, 53, 10344-10347	3.3	50
63	Stability of subsurface oxygen at Rh(111). *Physical Review B*, **2002**, 65,	3.3	49
62	Vanadium oxides on aluminum oxide supports. 1. Surface termination and reducibility of vanadia films on alpha-Al2O3(0001). *Journal of Physical Chemistry B*, **2005**, 109, 23523-31	3.4	41
61	Partial oxidation of methanol on well-ordered V(2)O(5)(001)/Au(111) thin films. *Physical Chemistry Chemical Physics*, **2009**, 11, 3290-9	3.6	40
60	The non-innocent role of cerium oxide in heterogeneous catalysis: A theoretical perspective. *Catalysis Today*, **2015**, 253, 20-32	5.3	39
59	Experimental and Theoretical Study on the Nature of Adsorbed Oxygen Species on Shaped Ceria Nanoparticles. *Journal of Physical Chemistry Letters*, **2018**, 9, 6593-6598	6.4	38
58	Insights into the Nature of Formate Species in the Decomposition and Reaction of Methanol over Cerium Oxide Surfaces: A Combined Infrared Spectroscopy and Density Functional Theory Study. *Journal of Physical Chemistry C*, **2015**, 119, 21452-21464	3.8	35
57	Crystal structure and vibrational spectra of AlVO4. A DFT study. *Journal of Physical Chemistry B*, **2005**, 109, 394-400	3.4	34
56	Electronic properties and charge state of gold monomers and chains adsorbed on alumina thin films on NiAl(110). *Physical Review B*, **2010**, 81,	3.3	31
55	Electron correlations in the ground state of silicon. *Physical Review B*, **1989**, 39, 5156-5164	3.3	30
54	Unraveling the oxygen vacancy structures at the reduced CeO2(111) surface. *Physical Review Materials*, **2018**, 2,	3.2	30
53	Adlayer Core-Level Shifts of Random Metal Overlayers on Transition-Metal Substrates. *Physical Review Letters*, **1997**, 78, 1807-1810	7.4	28
52	Surface Stabilizes Ceria in Unexpected Stoichiometry. *Journal of Physical Chemistry C*, **2017**, 121, 6844-6851	3.3	27

51	Vanadium oxides on aluminum oxide supports. 2. Structure, vibrational properties, and reducibility of V2O5 clusters on alpha-Al2O3(0001). *Journal of Physical Chemistry B*, **2005**, 109, 23532-42	3.4	26
50	Identification of single-atom active sites in CO oxidation over oxide-supported Au catalysts. *Journal of Catalysis*, **2020**, 383, 264-272	7.3	25
49	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable Al2O3(001) Compared to Al2O3(0001). *Journal of Physical Chemistry C*, **2007**, 111, 5141-5153	3.8	25
48	Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(). *Surface Science*, **2003**, 522, 185-197	1.8	25
47	Hydrogen Spillover to Copper Clusters on Hydroxylated Al2O3. *Journal of Physical Chemistry C*, **2018**, 122, 18445-18455	3.8	24
46	Diffusion Barriers Block Defect Occupation on Reduced CeO_{2}(111). *Physical Review Letters*, **2016**, 116, 236101	7.4	23
45	Dry Reforming of Methane on a Highly-Active Ni-CeO2 Catalyst: Effects of Metal-Support Interactions on CH Bond Breaking. *Angewandte Chemie*, **2016**, 128, 7581-7585	3.6	23
44	Oxygen-Vacancy Dynamics and Entanglement with Polaron Hopping at the Reduced CeO_{2}(111) Surface. *Physical Review Letters*, **2019**, 122, 096101	7.4	22
43	Ni Nanoparticles on CeO2(111): Energetics, Electron Transfer, and Structure by Ni Adsorption Calorimetry, Spectroscopies, and Density Functional Theory. *ACS Catalysis*, **2020**, 10, 5101-5114	13.1	22
42	Vanadia Aggregates on an Ultrathin Aluminum Oxide Film on NiAl(110). *Journal of Physical Chemistry C*, **2010**, 114, 4983-4994	3.8	20
41	Electronic correlations of cubic boron nitride. *Physical Review B*, **1991**, 44, 3526-3536	3.3	20
40	The Structure of Oxygen Vacancies in the Near-Surface of Reduced CeO (111) Under Strain. *Frontiers in Chemistry*, **2019**, 7, 436	5	18
39	In Situ and Theoretical Studies for the Dissociation of Water on an Active Ni/CeO2 Catalyst: Importance of Strong MetalSupport Interactions for the Cleavage of OH Bonds. *Angewandte Chemie*, **2015**, 127, 3989-3993	3.6	18
38	Methanol Adsorption on V2O3(0001). *Topics in Catalysis*, **2011**, 54, 669-684	2.3	18
37	Vanadia and Water Coadsorption on Tetragonal Zirconia Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 18191-18203	3.8	17
36	Reduction of the (001) surface of gamma-V2O5 compared to alpha-V2O5. *Journal of Physical Chemistry B*, **2005**, 109, 374-80	3.4	17
35	The structure of epitaxial V2O3 films and their surfaces: A medium energy ion scattering study. *Surface Science*, **2012**, 606, 1716-1727	1.8	16
34	Nucleation of gold atoms on vanadyl-terminated V2O3(0001). *New Journal of Physics*, **2009**, 11, 093007	2.9	15

33	Orbital and dipolar contributions to the hyperfine fields in bulk bcc Fe, hcp Co, and at the Fe/Ag(100) interface: The inclusion of orbital polarization. *Physical Review B*, **2001**, 63,	3.3	14
32	Publisher's Note: Hybrid functionals applied to rare-earth oxides: The example of ceria [Phys. Rev. B 75, 045121 (2007)]. *Physical Review B*, **2007**, 75,	3.3	13
31	Breaking Simple Scaling Relations through Metal-Oxide Interactions: Understanding Room-Temperature Activation of Methane on M/CeO (M = Pt, Ni, or Co) Interfaces. *Journal of Physical Chemistry Letters*, **2020**, 11, 9131-9137	6.4	13
30	Single Ni Sites Supported on CeO2(111) Reveal Cooperative Effects in the Water□as Shift Reaction. *Journal of Physical Chemistry C*, **2019**, 123, 7749-7757	3.8	13
29	Do Au Atoms Titrate Ce3+Ions at the CeO2□(111) Surface?. *Journal of Physical Chemistry C*, **2016**, 120, 927-933	3.8	12
28	Reaction Pathway for Coke-Free Methane Steam Reforming on a Ni/CeO Catalyst: Active Sites and the Role of Metal-Support Interactions. *ACS Catalysis*, **2021**, 11, 8327-8337	13.1	12
27	Controlled selectivity for ethanol steam reforming reaction over doped CeO2 surfaces: The role of gallium. *Applied Catalysis B: Environmental*, **2020**, 277, 119103	21.8	10
26	Electronic structure of random Ag-Pd and Ag-vacancy overlayers on an fcc Pd(001) substrate. *Physical Review B*, **1993**, 48, 1870-1876	3.3	10
25	Metal-Support Interactions and C1 Chemistry: Transforming Pt-CeO into a Highly Active and Stable Catalyst for the Conversion of Carbon Dioxide and Methane. *ACS Catalysis*, **2021**, 11, 1613-1623	13.1	10
24	Theoretical Study of the Catalytic Performance of Activated Layered Double Hydroxides in the Cyanoethylation of Alcohols. *Journal of Physical Chemistry C*, **2019**, 123, 8777-8784	3.8	9
23	Oxygen Defects at Reducible Oxide Surfaces: The Example of Ceria and Vanadia. *Springer Series in Surface Sciences*, **2015**, 149-190	0.4	9
22	Nature of the Active Sites on Ni/CeO Catalysts for Methane Conversions. *ACS Catalysis*, **2021**, 11, 10604-10613	13.1	9
21	Enhanced oxidation activity from modified ceria: MnOx□eria, CrOx□eria and Mg doped VOx□eria. *Applied Catalysis B: Environmental*, **2016**, 197, 313-323	21.8	8
20	Comment on □Oxygen Vacancy Ordering and Electron Localization in CeO2: Hybrid Functional Study□*Journal of Physical Chemistry C*, **2017**, 121, 21080-21083	3.8	8
19	Insight into the mechanism of the water-gas shift reaction over Au/CeO catalysts using combined operando spectroscopies. *Faraday Discussions*, **2021**, 229, 232-250	3.6	8
18	In Situ Investigation of Methane Dry Reforming on Metal/Ceria(111) Surfaces: Metal□Support Interactions and C□H Bond Activation at Low Temperature. *Angewandte Chemie*, **2017**, 129, 13221-13226	3.6	7
17	First-principles study of hyperfine fields in a Cd impurity in the Fe/Ag(100) interface. *Physical Review B*, **2001**, 64,	3.3	7
16	Interference, resonances, and bound states at the Pd(001) and Rh(001) surfaces. *Physical Review B*, **1994**, 50, 11142-11145	3.3	7

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15	Relative Stability of Near-Surface Oxygen Vacancies at the CeO2(111) Surface upon Zirconium Doping. *Journal of Physical Chemistry C*, **2020**, 124, 625-638	3.8	7
14	Toward an Atomic-Level Understanding of Ceria-Based Catalysts: When Experiment and Theory Go Hand in Hand. *Accounts of Chemical Research*, **2021**, 54, 2884-2893	24.3	7
13	Vibrational Frequencies of Cerium-Oxide-Bound CO: A Challenge for Conventional DFT Methods. *Physical Review Letters*, **2020**, 125, 256101	7.4	6
12	Reduced CeO2(111) ordered phases as bulk terminations: Introducing the structure of Ce3O5. *Physical Review Materials*, **2018**, 2,	3.2	6
11	Interaction of HCl with a CeO2(111) Layer Supported on Ru(0001): A Theory and Experiment Combined Study. *Journal of Physical Chemistry C*, **2018**, 122, 19584-19592	3.8	4
10	Imaging of individual adatoms on oxide surfaces by dynamic force microscopy. *Physical Review B*, **2010**, 81,	3.3	4
9	Nonuniform temperature dependence of the reactivity of disordered VO(x)/kappa-Al2O3(001) surfaces: a density functional theory based Monte Carlo study. *Journal of Chemical Physics*, **2008**, 129, 224710	3.9	4
8	Elucidating the Oxygen Storage-Release Dynamics in Ceria Nanorods by Combined Multi-Wavelength Raman Spectroscopy and DFT. *Journal of Physical Chemistry Letters*, **2020**, 11, 8554-8559	6.4	4
7	Ce=O Terminated CeO. *Angewandte Chemie - International Edition*, **2021**, 60, 13835-13839	16.4	3
6	The electronic structure of a model bimetallic catalyst: symmetry-resolved density of states at □G for Cu/Ru(111). *Surface Science*, **1995**, 331-333, 716-722	1.8	1
5	Overlayer and interface resonances and bound states at Pd/Ag(001)and Ag/Pd(001) surfaces. *Surface Science*, **1995**, 331-333, 691-696	1.8	1
4	Ce=O Terminated CeO2. *Angewandte Chemie*, **2021**, 133, 13954-13958	3.6	1
3	Chemical Reactivity Theory for Physicists; A Work in Progress. *Kluwer International Series in Engineering and Computer Science*, **1996**, 315-333		0
2	Adiabatic limit for the time dependent Coulomb problem. *Journal of Chemical Physics*, **1986**, 84, 3324-3326	3.9	
1	Enhanced Methanol Production over Non-promoted Cu□MgO□Al2O3 Materials with Ex-solved 2 nm Cu Particles: Insights from an Operando Spectroscopic Study. *ACS Catalysis*, **2022**, 12, 3845-3857	13.1	